MR308 Jan 3:0

Computational Modeling of Materials

Instructor

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Department: MRC

Course Time: Tue., Thu., 9:00 - 10:30 AM

Lecture venue: MRC Seminar hall

Detailed Course Page:

Announcements

The first meeting of "MR308 Computational Modeling of Materials"

will take place on 2nd of January 2018 at MRC Seminar Hall at

9:00 AM.

Timings: 9:00 AM-10:30 AM on Tuesday and Thursday.

We can discuss other details during the meeting.

Brief description of the course

This is an entirely new course, which was conceived and designed by Dr. Singh. In this course, the various quantum mechanical methods to solve the many-body problems are covered in great depth. Very few courses having a similar syllabus as this course are offered in India, making this course one of its kind. The course is divided into two modules: theory and hands-on sessions. The intention behind such compartmentalization is that whatever is taught in theory is instantly visible through practical exercises in the hands-on sessions making it easier for students to understand.

The course takes the students through a chronological development from tight binding and Thomas-Fermi theory to all the way to density functional theory and other many-body approaches.The course starts with the tight-binding method of representing wavefunctions as a linear combination of atomic orbitals, and then systematically moves to density functional theory (DFT).

In the hands-on sessions, the students get a flavor of how DFT is used in a practical application. Given the diverse aspects of this course, students from different disciplines (sciences, engineering) attend the course. Earlier, this course was allowed only for the graduate students, given its advanced syllabus. However, more recently there has been an increase in the strength of undergraduate students crediting it and excelling in it.

Prerequisites

Basic quantum mechanics

Syllabus

Introduction to computational modeling of materials, Description of atomic interaction, Tight binding approximation, Hartree-Fock, Molecular Orbital Method, Density functional theory, Applications of these methods in modeling of mechanical, electronic, magnetic, optical, and dielectric properties of materials, Design principles of novel materials

Course outcomes

Students who have taken the previous course have immensely benefited from this course, there have been many other students, who, without any prerequisite knowledge of quantum mechanics, statistical mechanics etc. have grasped the underlying concepts and have successfully applied the learning from this course to their research work.

Grading policy

10% Assignments 40% mid-term, 40% final, 10% project

Assignments

Resources